2. Fonctions de corrélation

2.3 Propriétés générales

- Kramers - Krönig
- $\omega \chi''$ et dissipation
- F.-D.
- Règles de somme

$$\chi^{R}_{BA}(t-t') = \frac{i}{\hbar}\langle [B(t), A(t')]\rangle \Theta(t-t')$$

$$\rightarrow \quad = 2i\,\chi''_{BA}(t-t')\,\Theta(t-t')$$

$$\boxed{\chi''_{BA} = \frac{1}{2\hbar}\langle [B(t), A(t')]\rangle}$$

$\vec{r} \rightarrow -\vec{r}$ $\quad \chi''_{BA}(q, t-t') = \epsilon^{P}_{B}\epsilon^{P}_{A}\chi''_{BA}(-q, t-t')$

$t \rightarrow -t$ $\quad \chi''_{A_i A_j}(\omega) = \epsilon^{t}_{A_i}\epsilon^{t}_{A_j}\chi''_{A_j A_i}(\omega)$

Commutateur:

$$\int d(t-t')\, \underbrace{e^{-i\omega(t-t')}}$$

$$\chi''_{A_i A_j}(t-t') = -\chi''_{A_j A_i}(t'-t)$$

$$\boxed{\chi''_{A_i A_j}(\omega) = -\chi''_{A_j A_i}(-\omega)}$$

Hermiticité:

$$\chi''_{A_i A_j}(t-t') = \left[\chi''_{A_j A_i}(t'-t)\right]^*$$

$$\boxed{\chi''_{A_i A_j}(\omega) = \chi''^{*}_{A_j A_i}(\omega)}$$

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Preuve $\langle\psi|A|\varphi\rangle^* = \langle\varphi|A^+|\psi\rangle$

$$= \langle\varphi|A|\psi\rangle$$

$$\langle i|\rho A_i A_j|i\rangle^*$$

$$= \langle i|A_j A_i \rho|i\rangle$$

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e.g. $\chi''_{\rho_q \rho_{-q}}(\omega) = -\chi''_{\rho_q \rho_{-q}}(-\omega)$

$$\rightsquigarrow \chi''_{\rho_q \rho_{-q}}(\omega) = \left[\chi''_{\rho_q \rho_{-q}}(+\omega)\right]^*$$

$$\chi''_{\rho_r \rho_{r'}}(\omega) = -\chi''_{\rho_{r'} \rho_r}(-\omega)$$

$$= -\chi''_{\rho_r \rho_{r'}}(-\omega)$$

$\boxed{\text{K. K.}}$ causalité

$$\mathrm{Re}\,\chi^R_{A_iA_j}(\omega) = \mathcal{P}\int \frac{d\omega'}{\pi} \frac{\mathrm{Im}\,\chi^R_{A_iA_j}(\omega')}{\omega'-\omega}$$

$$\mathrm{Im}\,\chi^R_{A_iA_j}(\omega) = -\mathcal{P}\int \frac{d\omega'}{\pi} \frac{\mathrm{Re}\,\chi^R_{A_iA_j}(\omega')}{\omega'-\omega}$$

$$\chi^R_{A_iA_j}(t-t') = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\, e^{-i\omega(t-t')}\, \chi^R_{A_iA_j}(\omega)$$

$$\| \qquad\qquad\qquad\qquad\qquad \downarrow$$

0 si $t-t' < 0$

Analytique pour $\mathrm{Im}(\omega) > 0$

$$\int_{C'} \frac{d\omega'}{\pi} \frac{1}{\omega' - \omega - i\eta} \chi^{R}_{A_i A_j}(\omega') = 2i \chi^{R}_{A_i A_j}(\omega + i\eta)$$

$$\int_{C} = 0$$

$$\omega' = R e^{i\theta}$$

$$d\omega' = R\, i\, d\theta\, e^{i\theta}$$

$$\lim_{\eta \to 0} \frac{1}{\omega \pm i\eta} = \lim_{\eta \to 0} \frac{\omega \mp i\eta}{\omega^2 + \eta^2}$$

$$= \lim_{\eta \to 0} \left(\frac{\omega}{\omega^2 + \eta^2} \mp i \frac{\eta}{\omega^2 + \eta^2} \right)$$

$$\lim_{\eta \to 0} \frac{1}{\omega \pm i\eta} = \mathcal{P}\left(\frac{1}{\omega}\right) \mp i\pi\delta(\omega)$$

$$\int \frac{d\omega'}{\pi} \frac{1}{\omega'-\omega-i\eta} \chi^R_{A_iA_j}(\omega') = 2i\, \chi^R_{A_iA_j}(\omega)$$

$$\left[P \int \frac{d\omega'}{\pi} \frac{1}{\omega'-\omega} \chi^R_{A_iA_j}(\omega') \right]$$

$$P \int \frac{d\omega'}{\pi} \frac{1}{\omega'-\omega} \mathrm{Im}\, \chi^R_{A_iA_j}(\omega') = \mathrm{Re}\, \chi^R_{A_iA_j}$$

$$= i\, \chi^R_{A_iA_j}$$

Autre preuve:

$$\chi^{R}_{A_i A_j}(\omega) = 2i \int \frac{d\omega'}{2\pi} \chi''_{A_i A_j}(\omega') \theta(\omega-\omega')$$

$$\int_{-\infty}^{\infty} dt\, e^{i\omega t} \theta(t) = \frac{e^{i\omega t}}{i\omega} \Big|_{0}^{\infty}$$

$$\int_{-\infty}^{0} dt'\, e^{i\omega t'} = \frac{e^{i\omega t'}}{i\omega} \Big|_{0}^{\infty}$$

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Appliquer le champ externe

avec $e^{\eta t'}$ $\quad t' \to -\infty$

À $t = \infty$ réponse = 0

$$e^{-\eta t}$$

$$\boxed{\int d(t-t')\, e^{i\omega(t-t')}}$$

$$\chi^R_{A_i A_j}(t-t')\, e^{-\eta(t-t')}$$

$$= 2i\chi''_{A_i A_j}(t-t')\,\theta(t-t')\, e^{-\eta(t-t')}$$

$$\chi^R_{A_iA_j}(\omega+i\eta) = -\cancel{2i}\int \frac{d\omega'}{\cancel{2}\pi}\,\frac{\chi''_{A_iA_j}(\omega')}{\cancel{i}(\omega+i\eta-\omega')}$$

$$\boxed{\chi^R_{A_iA_j}(\omega) = \int \frac{d\omega'}{\pi}\,\frac{\chi''_{A_iA_j}(\omega')}{\omega'-\omega-i\eta}}$$

Représentation spectrale.

$$\chi_{A_i A_j}(z) = \int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{\chi''_{A_i A_j}(\omega')}{\omega' - z}$$

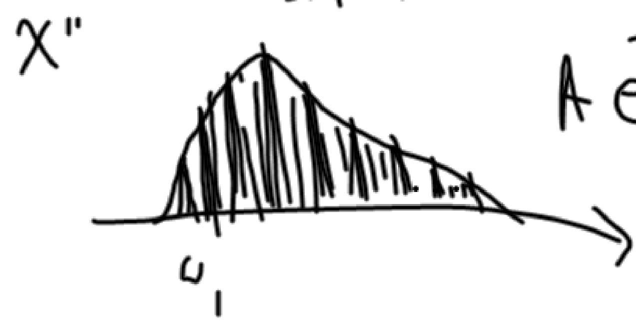
$$\chi^R_{A_i A_j} = \lim_{\eta \to 0} \chi_{A_i A_j}(z) \Big|_{z = \omega + i\eta}$$

$$\chi^A_{A_i A_j} = \lim_{\eta \to 0} \chi_{A_i A_j}(z) \Big|_{z = \omega - i\eta}$$

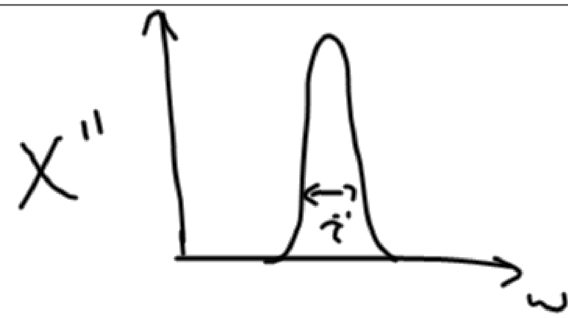
$$\chi_{A_iA_j}(\omega+i\eta) - \chi_{A_iA_j}(\omega-i\eta)$$

$$= 2i\,\chi''_{A_iA_j}(\omega)$$

Irréversibilité.



$$A e^{-i\omega_1(t-t')} + B e^{-i\omega_2(t-t')} + \cdots$$



$$\chi \to e^{-t/\tau}$$

$$V \to \infty \quad \text{(volume)}$$

$$\eta \to 0 \quad \text{ensuite.}$$

Positivity of $\omega \chi''$ + dissipation.

$$\frac{dW}{dt} = \frac{d\, \delta H(t)}{dt} = -\int d^3r\, A_i(r)\, \frac{d a_i(\vec{r},t)}{dt}$$

$$= -A_i \frac{d a_i(t)}{dt}$$

$$\left\langle \frac{dW}{dt} \right\rangle = -\left[\langle A_i \rangle + \langle \delta A_i \rangle \right] \frac{d a_i}{dt}.$$

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$$\overline{W} = -\int_{-T/2}^{T/2} dt \, \langle \delta A_i(t) \rangle \frac{d a_i(t)}{dt} > 0$$

$$= -\int \frac{d\omega}{2\pi} \langle \delta A_i(\omega) \rangle \, i\omega \, a_i(-\omega)$$

$$= -\int \frac{d\omega}{2\pi} \, \underline{a_i(-\omega)} \, \chi^R_{A_i A_j}(\omega) \, i\omega \, a_j(\omega)$$

$$> 0$$

$$\overline{W} = -\frac{1}{2}\int \frac{d\omega}{2\pi}\, a_i(-\omega)\left[\chi^R_{A_iA_j}(\omega) - \chi^R_{A_jA_i}(-\omega)\right]$$

$$i\omega\, a_j(\omega) > 0$$

$$\chi^R_{A_iA_j}(\omega) - \chi^R_{A_jA_i}(-\omega) = 2i\,\chi''_{A_iA_j}(\omega)$$

$$= \int \frac{d\omega'}{\pi}\left(\frac{\chi''_{A_iA_j}(\omega')}{\omega' - \omega - i\eta} - \frac{\chi''_{A_iA_j}(+\omega')}{+\omega' - \omega + i\eta}\right)$$

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$$\int \frac{d\omega}{2\pi}\, a_i^*(\omega)\, \chi''_{A_iA_j}(\omega)\, a_j(\omega) > 0$$

$$\left[\int e^{i\omega t} \varphi(t)\, dt\right]^*$$

$$= \int e^{-i\omega t} \varphi(t)\, dt$$

Soit une seule fréquence pour a_i

$$a_i^*(\omega)\, \chi''_{A_iA_i}(\omega)\, \omega\, a_i(\omega) > 0$$

Matrice

$$\boxed{\omega\, \chi''_{A_iA_i}(\omega) > 0}$$

$\chi''_{A_iA_j}(\omega)\,\omega$ est positive définie.

Théorème de fluctuation dissipation

$$S_{A_iA_j}(t) = \left\langle \left(A_i(t) - \langle A_i \rangle\right)\left(A_j(0) - \langle A_j \rangle\right)\right\rangle$$

$$= \langle A_i(t) A_j(0) \rangle - \langle A_i \rangle \langle A_j \rangle$$

$$S_{A_iA_j}(t) = \langle \delta A_i(t)\, \delta A_j \rangle$$

À prouver :

$$\boxed{S_{A_iA_j}(\omega) = \frac{2\hbar}{1-e^{-\beta\hbar\omega}}\chi''_{A_iA_j}(\omega)}$$

Preuve : $\chi''_{A_iA_j}(t) = \frac{1}{2\hbar}\langle[A_i(t), A_j]\rangle$

$$= \frac{1}{2\hbar}\langle[\delta A_i(t), \delta A_j]\rangle$$

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$$= \frac{1}{2\hbar}\Big(S_{A_iA_j}(t) - S_{A_iA_j}(t-i\hbar\beta)\Big)$$

$$\boxed{S_{A_jA_i}(-t) = S_{A_iA_j}(t-i\hbar\beta)}$$

$$\boxed{S_{A_jA_i}(-\omega) = e^{-\beta\hbar\omega}\, S_{A_iA_j}(\omega)}$$

Bilan détaillé

$$S_{A_j A_i}(-t) = \frac{1}{Z} T_r \left[e^{-\beta H} \delta A_j(-t) \delta A_i \right]$$

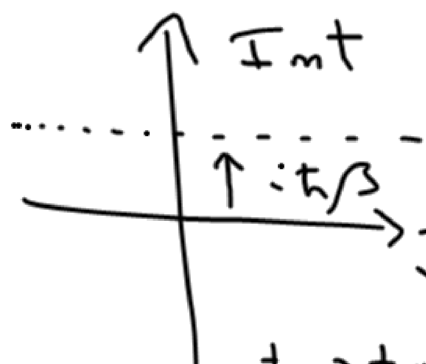
$$e^{-iHt/\hbar} \delta A_j e^{iHt/\hbar}$$

$$= \frac{1}{Z} T_r \left[e^{-\beta H} \delta A_j \delta A_i(t) \right]$$

$$= \frac{1}{Z} T_r \left[e^{-\beta H} e^{\beta H} e^{iHt/\hbar} \delta A_i e^{-iHt/\hbar} e^{-\beta H} \delta A_j \right]$$

$$= S_{A_i A_j}(t - i\hbar\beta)$$

$$\int_{-\infty}^{\infty} dt\, e^{i\omega t}\, S_{A_i A_j}(t - i\hbar\beta)$$



$$\int_{-\infty}^{\infty} dt\, e^{i\omega(t + i\hbar\beta)}\, S_{A_i A_j}(t)$$

$t \to t + i\hbar\beta$

$$= e^{-\beta\hbar\omega}\, S_{A_i A_j}(\omega)$$

$$S_{A_i A_j}(t - i\hbar\beta) = e^{-i\hbar\beta \frac{\partial}{\partial t}} S_{A_i A_j}(t)$$

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$$S_{A_j A_i}(-\omega$$

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